

alpha-Humalene

6753-98-6 | DTXSID30858793

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -80.6 °C

Global applicability domain: Inside

Local applicability domain index: 8.77e-01

Confidence level: 6.28e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,5-Cyclooctadiene

Measured: -56.4

Predicted: -68.8

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Cyclopentene

Measured: -135

Predicted: -124

[Image not found](#)

Cyclohepta-1,3-diene

Measured: -110

Predicted: -75.9

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Cycloheptene

Measured: -56.0

Predicted: -84.4